On recombination in strong laser fields: effect of a slow drift

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The dynamics of the recombination in ultrastrong atomic fields is studied for one-dimensional models by numerical simulations. A nonmonotonic behavior of the bound state final population as a function of the laser field amplitude is examined. An important role of a slow drift of an electron wave packet is observed.

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I. INTRODUCTION

It is well known that during atomic photoionization in ultrastrong laser fields a peculiar effect occurs: for a given pulse length an interval of field intensities exists in which the ionization probability is a decreasing function of the field intensity. This is called adiabatic atomic stabilization against photoionization [1, 2]. The motivation of the present work is to look for a similar effect in the inverse process, namely atomic recombination in ultrastrong fields. The main difference between these processes is due to different initial conditions. The process of strong-field recombination has recently been examined by Hu and Collins [3], who however investigated the dependence of the process on the initial momentum of the incoming electron.

During the recombination one should expect dynamical effects similar to those observed in the case of ionization. As it has been shown in the works devoted to the atomic stabilization, in laser fields of order of a few atomic units most of the electron wave packet moves as a whole, performing oscillations in the rhythm of the field. Additionally, long time oscillations of the packet are possible which are due to an asymmetry of the interaction of its different parts with the binding potential; in our earlier papers [4, 5, 6] we have called them a slow drift. The slow drift has the range equal to that of the classical oscillations of a free electron in the laser field and it was possible to give an analytic formula for its frequency in the case of the binding potential being a rectangular well. The fact that a significant part of the packet moves without changing of its shape, in particular of its width, can be explained in terms of the so-called Kramers-Henneberger (KH) well, which is the mean potential (zero-th term of the Fourier expansion) of the oscillating nucleus in the electron's reference frame. The stabilization of the wavepacket can be interpreted as its trapping in the eigenstate of the KH well. In the laboratory frame the KH well oscillates in the rhythm of the laser field and may also perform the slow drift, which was described by a generalized model of Ref. [4]. For longer times a decay of the KH state can be observed, due to an influence of higher terms of the above-mentioned Fourier expansion, and the corresponding decay rate has been evaluated [7]. The probability of finding the electron in the atomic bound state is thus a complicated function of time, which reflects a rapid oscillatory motion, a slow drift and a finite lifetime of the KH eigenstate. Moreover, a necessary condition for the stabilization to occur is that the pulse have such a shape that the corresponding electron classical trajectory should remain in the neighborhood of the nucleus.

In this work we present the results of numerical simulations of the dynamics of recombination for two model one-dimensional systems: a rectangular potential well and a long-range Coulomb-like potential. We will examine the time dependence of the bound state population (initially equal to zero) and the dynamics of the wave packet. As the measure of efficiency of recombination we take the final population of the bound state. In particular we study how the details of the dynamics depend on the amplitude of the laser field and as a consequence on the details of the slow drift.

II. NUMERICAL APPROACH

Strong-field recombination has been investigated in which an initially free electron modeled by a Gaussian packet, intially resting at twice the amplitude of classical free oscillations, is carried towards the ion in the laser field. The ion has been modeled by two kinds of a binding potential.

The dynamics of recombination has been examined by numerically solving the time-dependent Schrödinger equation in one spatial dimension. The computations have been performed on a grid of 16384 points. The space covered by our grid extends from -100 to 100 a.u. (the grid step is about 0.0122 a.u.). Calculations have been performed for two atomic models: the rectangular symmetrical well and a soft core atom potential. The rectangular well

$$V(x) = -V_1 \Theta(|a_1 - x|) \tag{1}$$

of the depth equal to $V_1 = 2.049$ a.u. and half-width equal to $a_1 = 0.122$ a.u. is placed in the middle of the

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simulation space. The function Θ is the Heaviside step function. The same well parameters were earlier used in the studies of stabilization [4]. We have also used the model atom potential proposed by Eberly *et al.* [8]:

$$V(x) = -\frac{1}{\sqrt{1+x^2}}. \quad (2)$$

To simulate the evolution of a one-dimensional wavefunction we use the Crank-Nicholson scheme, which for Schrödinger equation leads to the often used symmetrical Cayley's formula [9]. The simulations have been performed in the dipole approximation in the length gauge, i.e. the Hamiltonian of the system reads (in atomic units)

$$\hat{H} = -\frac{1}{2}\frac{\partial^2}{\partial x^2} + V(x) + x \cdot \varepsilon(t), \quad (3)$$

where the laser electric field $\varepsilon(t) = \varepsilon_0\Theta(t)\Theta(t_f - t)\cos(\omega t - \pi)$ is directed along the x-axis and acts only during the time interval t_f. The period of the laser is $T = 2\pi/\omega$, where $\omega = 1$ a.u. is the laser frequency. We have changed the laser field amplitude ε_0 in the range between 1 to 15 a.u. The time step was equal to $\Delta t = T/10^4$. The convergence of the computer simulations has been checked on the grid with 65536 spatial nodes and alternatively with a ten-times smaller time step. No important differences have been visible.

The initial position of the wavepacket, initially taken to be Gaussian $|\psi|^2 = \exp[-(x-x_0)^2/(2\delta^2)]$ with the variance $\delta^2 = 0.25$ a.u., has been prepared very carefully, independently for each simulation. The main condition is that the electron should be placed over the well after the first half of the period, i.e. $\bar{x}(T/2) = 0$, $\bar{x}$ being the packet's center of mass. Moreover, we require it to have at that time zero velocity to make the recombination more probable. This is why we have chosen the packet's initial position $x_0 = -2\varepsilon_0/\omega^2$ and initial velocity equal to zero so that the first classical turning point of a free oscillation occurs over the well. Note that the dependence of the recombination efficiency on the initial packet velocity has already been the subject of investigations of Ref. [3].

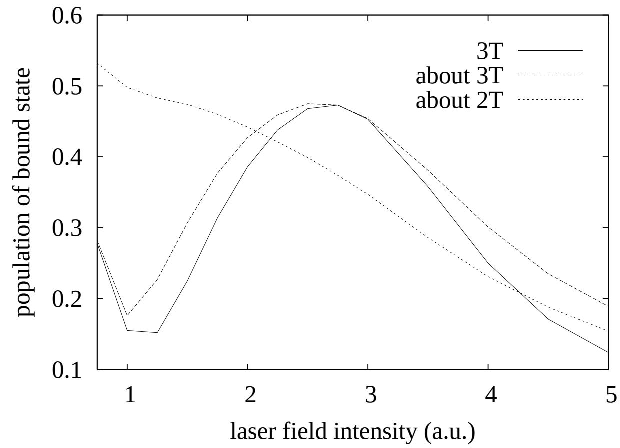

FIG. 1: The population of the ground state in the model atomic potential in the recombination process as a function of the field intensity ε_0 in the case of the field being switched off at exactly $3T$, solid line; at the time instant of a maximum population in the vicinity of $3T$ (see comment in the text), dashed line; at the time instant of a maximum population in the vicinity of $2T$, short-dashed line.

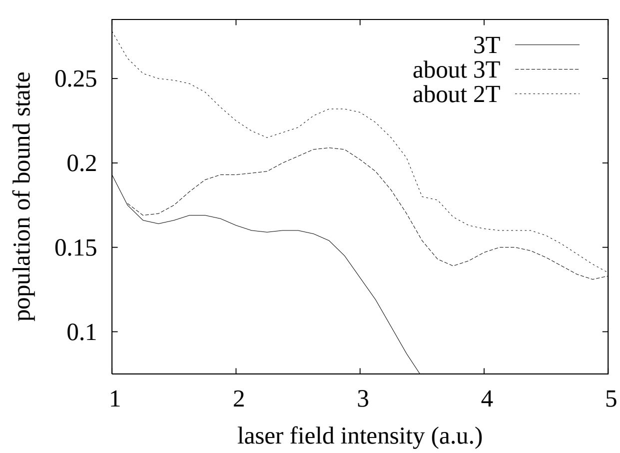

FIG. 2: As in Fig. 1 but for an only bound state of a well potential

III. RESULTS AND INTERPRETATION

In the case of the recombination process one observes a nonmonotonic dependence of the bound state population on the field intensity. It is well visible in Fig. 1 where the ground state population is shown as a function of the field intensity. In each case the rectangular pulse has been switched off at the time instant closest to three optical periods ($3T$) at which the ground state population exhibits a maximum (except for the solid line which has been obtained exactly at $3T$). At the time $2T$ the maximum is not yet formed. A wide maximum is seen for $\varepsilon_0 \approx 2.5$ a.u. both for the pulse duration of exactly $3T$ and approximately $3T$. A similar nonmonotonicity is observed in the case of a potential well (see Fig. 2). The figure suggests an existence of even more maxima which are however less pronounced for short times. This is confirmed for longer pulses in Fig. 3 (upper plot) in which one can see two separated maxima, one of which occurs for $\varepsilon_0 \approx 2.5$ a.u. for all pulse lengths, while the other one, being wider, shifts slowly for increasing pulse lengths. The origin of the peaks is different. The left peak can be attributed to a long lifetime τ of the eigenstate of the Kramers-Henneberger well; according to Ref. [7] τ exhibits a maximum for such ε_0 for which $J_1(\varepsilon_0\sqrt{2\omega}/\omega^2) = 0$, i.e ε_0 =2.71 a.u. and 4.96 a.u. (for the range of field amplitudes examined in this work). The position of the right hand side peak for different values of

the field intensity and of the pulse duration is evidently connected with the slow drift of the wave packet. A maximum is observed if at the moment of the field switch-off the slow drift of the main part of the packet is at such a stage that it is located at the well, which does not usually occur after an entire number of periods, and has a velocity close to zero. A similar field dependence of the bound state population can be seen in the case of the ionization (lower plot). Again one can see a peak for $\varepsilon_0 \approx 2.5$ a.u. for all the pulse durations and a second peak the position of which changes. One can also notice a small peak at about 5 a.u. (second minimum of J_1 and thus of $1/\tau$).

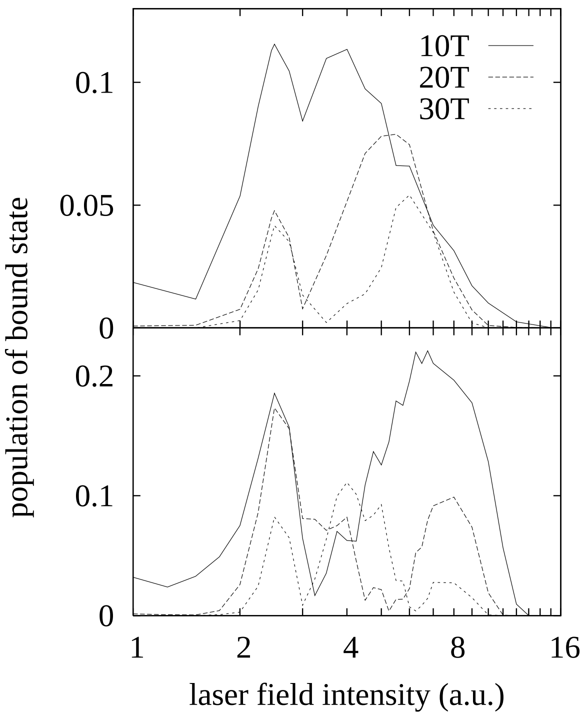

FIG. 3: The population of the bound state of the well potential in the recombination process (upper plot) and ionization process (lower plot) as functions of the field intensity ε_0 in the case of the field being switched off at exactly $10T$, $20T$ and $30T$.

In Figs 4 and 5 we show the evolution of the wave packet for different values of the field amplitude, for the potential well and for the model atom, respectively. For relatively small field amplitudes each field oscillation causes tearing the packet into smaller parts, typical of the regime of multiphoton ionization. For the field amplitude being of order of 2.5 a.u. one can already distinguish a main part of the packet, represented by the oscillating streak. A slow drift is imposed on the rapid oscillations with the field frequency ω. For the potential well the frequency of the slow oscillations may be evaluated using the formula $\Omega = \sqrt{2a_1V_1/(\sqrt{2\pi}\sigma^3)}$, where $\sigma = 2\varepsilon_0/\omega^2$ is the width of the wave packet trapped in the KH well [4]. Due to the slow drift, after an entire number of field periods, the packet ends up at different distances from the potential center, depending on the field amplitude.

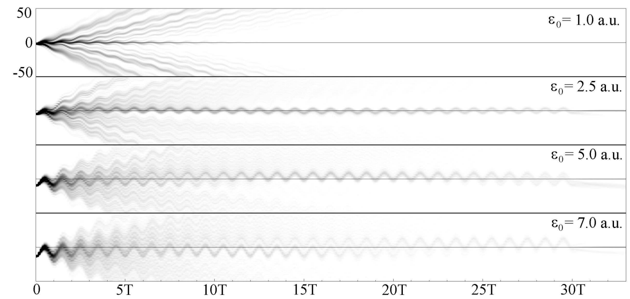

FIG. 4: The time evolution of the wave packet recombination in the well potential for different values of the field intensity. The level of blackening is proportional to the squared modules of the wave function.

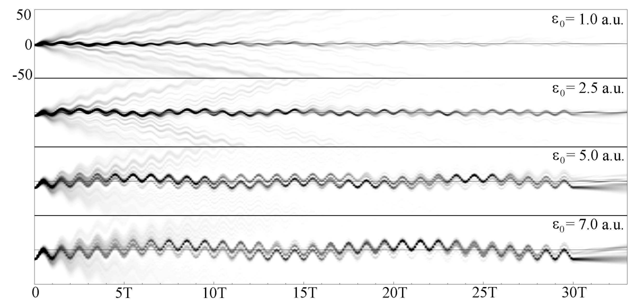

FIG. 5: As in Fig. 4 but for a model atomic potential.

The influence of the atomic potential is for our data stronger then in the case of the potential well, which is manifested by a larger frequency of the slow drift and a more effective recombination and population trapping (darker line) and less population thrown away as isolated small portions. In the case of the well potential, for large times the streak for $\varepsilon_0 = 2.5$ a.u. is significantly darker than for 2.0 a.u. and 3.0 a.u. (not shown), which corresponds to the first maximum of Fig. 3 (upper plot). There is also a correspondence between the level of population shown in Fig. 3 (upper plot) and the position of the streak of Fig. 4. For example for $t = 10T$ and $\varepsilon_0 = 5$ a.u. the streak is located at the position of the well $x = 0$ while for $\varepsilon_0 = 7$ a.u. its distance from the well is close to maximum due to the slow drift; this corresponds to the fact that the bound state population in Fig. 3 (upper plot) for $\varepsilon_0 = 5$ a.u. is larger than for $\varepsilon_0 = 7$ a.u. For $t = 30T$ the situation is reversed due to the slow drift.

For larger fields, especially in the case of atoms, the streak splits into two ones, which corresponds to population trapping in a superposition of two eigenstates of the KH well. One can also see a flow of the population from one streak to the other, which corresponds to the population oscillating between those two states. In the case of

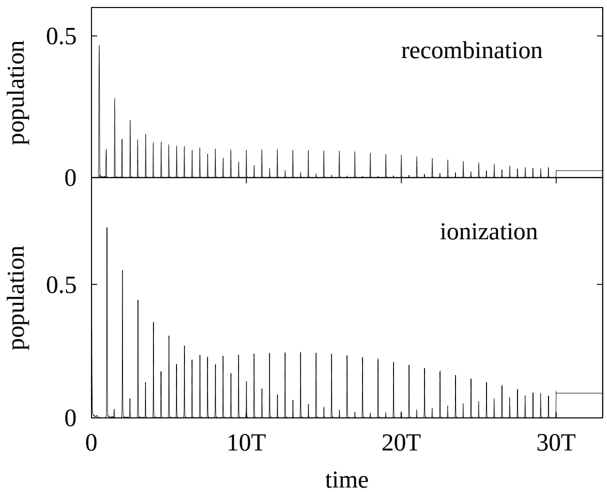

FIG. 6: The time evolution of the bound state population in the case of a well potential for the field intensity $\varepsilon_0 = 5$ a.u.

the rectangular well, for which an analytical form of the KH well is known [4], we have verified that for the field amplitude $\varepsilon_0 = 7$ a.u. there are indeed two eigenstates, the energy difference of which is approximately 0.016 a.u.; the corresponding period of oscillations agrees with the period of the population flow of Fig. 4.

The presence of the slow drift is reflected in the time dependence of the bound state population visible in Fig. 6. The maxima of the comb-like structure appear twice in each optical cycle at the time instants at which the packet's velocity is zero (turning points). The heights of the maxima depend on the current stage of the slow drift. The frequency of the exchange of the two families of the peaks, appearing respectively after an even or odd number of half-cycles, is the same, both in the case of ionization and recombination, as the frequency Ω of the slow drift, visible also in Fig. 4.

IV. CONCLUSIONS

A nonmonotonic behavior of the bound state final population as a function of the field amplitude has been observed in numerical simulations of strong-field recombination for one-dimensional models. The maxima may have two origins. First, they appear for such laser field intensities and pulse durations for which the packet ends up in such a stage of its rapid oscillations and of its slow drift that it is located at the nucleus and has zero velocity. Second, a maximum, located independently of the pulse duration, is due to a maximum lifetime of the KH bound state. For such fields that more than one KH state exist and are significantly populated, one additionally observes a third kind of oscillations of the wave packet (in addition to the oscillations with the optical frequency and the slow drift), which are due to the population oscillating between the KH eigenstates.

Acknowledgments

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